

An implicit relation between temperature and reaction rate in the SLFM

Jian Zhang,^{a)} Guowei He,^{b)} and Guodong Jin

LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

(Received 1 November 2010; accepted 28 November 2010; published online 10 January 2011)

Abstract The Arrhenius law implies that reaction rate is a continuous function of temperature. However, the steady laminar flamelet model (SLFM) does not explicitly give this functional relationship. The present study addresses this relation in the SLFM. It is found that reaction rate is not continuous in the mixture-fraction space. As a result, the SLFM is unable to predict local extinction and reignition. Furthermore, we use the unstable branch of the “S-curve” to fill the gap between steady burning branch and extinction one, and find that this modification leads to a continuous dependent of reaction rate on temperature. Thus the modified SLFM can describe the local extinction and reignition. © 2011 The Chinese Society of Theoretical and Applied Mechanics. [doi:10.1063/2.1101203]

Keywords nonpremixed turbulent combustion, local extinction and reignition, steady laminar flamelet model, unstable branch

Flamelet models are fundamentally important to turbulent combustion. The simplest and most frequently used flamelet model is the steady laminar flamelet model (SLFM). This model assumes that the reaction is quasisteady and consequently the transient effects can be neglected.^[1] Recently, many works have focused on the validation and improvement of the SLFM. Cuenot and Poinso^[2] investigated the applicability of the SLFM to turbulent nonpremixed combustion through direct numerical simulation (DNS) of flame-vortex interactions. They found that the SLFM becomes invalid when curvature, unsteadiness and quenching become important. Pitsch *et al.*^[3] used the unsteady flamelet model with Lagrangian time scale to discuss the transient effect in modeling diffusion flame. Claramunt *et al.*^[4] and Cònsul *et al.*^[5] analyzed the application of the SLFM in nonpremixed laminar flames and laminar partially premixed flames, and compared the SLFM with the unsteady laminar flamelet model. It was found that the SLFM is incapable of predicting unsteady reaction processes such as pollutant formation, local extinction and reignition, lift-off or blow-out. A widely accepted explanation is that unsteady processes can not be reasonably represented by the models which assume them to be steady.^[6]

The reaction rate provided by the SLFM controls the reaction process. According to the Arrhenius law the reaction rate has to be continuously dependent on temperature. However, the relation between temperature and reaction rate has not been explicitly stated in the SLFM. It remains unknown whether the Arrhenius law can be truly represented in the SLFM or not. In this study, this essential problem is addressed. We will give a new explanation on why the SLFM does not work in predicting local extinction and reignition. This explanation is helpful to further development of flamelet

models.

The functional relationship between temperature and reaction rate in the SLFM is investigated by the solutions of steady laminar flamelet equations. A single-step reversible reaction in a two-feed system is used. It is an extensively used, idealized chemical reaction model.^[1,2,7]

$$F_{\text{uel}} + rO_{\text{xidizer}} \rightleftharpoons (r+1)P_{\text{roduct}}. \quad (1)$$

Here r is the stoichiometric ratio meaning the mass of oxidizer required to react with a unit mass of fuel. Y_F , Y_O and Y_P stand for the mass fractions of fuel, oxidizer and product respectively. Thus the mixture fraction, a conserved scalar, is defined as

$$z = \frac{rY_F - Y_O + 1}{1 + r}, \quad (2)$$

which indicates the amount of mixing, having a value of unity in the fuel zone and zero in the oxidizer zone. On the other hand, the reduced temperature is defined as

$$\theta = \frac{T - T_u}{T_b - T_u}, \quad (3)$$

which is a chemically reactive scalar, indicating the progress of the reaction, varying between zero and unity. Here T is the local temperature of the flow field, T_b the adiabatic flame temperature and T_u the temperature of both the unburned fuel and oxidizer. An Arrhenius temperature dependent reaction scheme is used here. For simplicity, it is assumed that the molecular diffusivities of all species and of heat are equal. Consequently, the reduced temperature is identical to the mass fraction of product.^[8]

The relevant parameters of the Arrhenius reaction, such as the pre-exponential factor A , heat-release parameter α , Zeldovich number β and equilibrium constant K , are selected to make the reaction rate strongly temperature dependent.^[7] Their values are listed in Table 1. The values of α and β are taken close to those

^{a)}E-mail: zhangjian@lnm.imech.ac.cn

^{b)}Corresponding author. E-mail: hgw@lnm.imech.ac.cn.

Table 1. Numerical values of the thermochemistry parameters

r	A	α	β	K
1	8×10^4	0.87	4.0	100

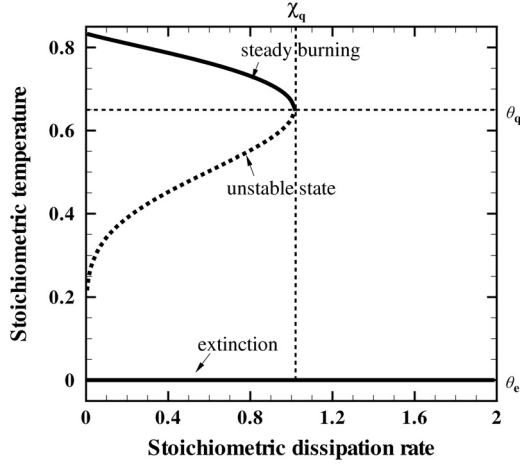


Fig. 1. The stoichiometric temperature is showed as a function of the stoichiometric dissipation rate of the mixture fraction. This curve is called “S-curve”. The “S-curve” represents the solutions of the steady flamelet equations under the present set of thermo-chemistry parameters.

used in the one-step chemistry models of hydrogen-oxygen reaction.^[9] Here $\alpha = (T_b - T_u)/T_b$, $\beta = T_a/T_b * \alpha$. In addition, T_a is the activation temperature. Therefore the reaction rate of the product can be written as follows

$$\omega_P = (r + 1)A \exp\left(\frac{-\beta}{\alpha}\right) \exp\left[\frac{-\beta(1 - Y_P)}{1 - \alpha(1 - Y_P)}\right] \times \left(Y_F Y_O - \frac{1}{K} Y_P^{r+1}\right). \quad (4)$$

The one-dimensional steady state flamelet equations are used to describe this chemical reaction. Assuming unity Lewis number, negligible Soret effect and radiation and neglecting the unsteady effect, the flamelet equations can be written as

$$\frac{\chi}{2} \frac{\partial^2 Y_i}{\partial z^2} + \omega_i = 0, \quad i = F, O, P. \quad (5)$$

Here, the instantaneous scalar dissipation rate is modeled by

$$\chi = \chi_{st} \exp[-2 \operatorname{erfc}^{-1}(2z)^2]. \quad (6)$$

Using Eq. (6) in the flamelet equations, the flamelet library can be constructed using two input parameters: z and χ_{st} . Here χ_{st} acts as an external parameter that is imposed on the flamelet structure by the mixture fraction field.^[5]

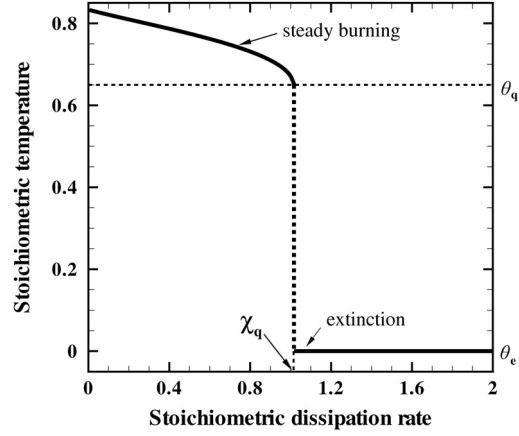


Fig. 2. This curve is extracted from the SLFM library, which is the combination of steady-burning branch and extinction line of solutions of steady laminar flamelet equations. Note the discontinuous jump between burning and extinguished solutions for $\theta_e < \theta_{st} < \theta_q$.

The flamelet equations (5) can be numerically solved using the program BVP4C in MATLAB.^[10] It can be seen from Fig. 1 that the complete set of their solutions consists of three branches, which form an “S-curve”. Here, χ_q denotes the quenching dissipation rate, θ_q the quenching temperature and θ_e the extinction temperature. The stoichiometric temperature and the stoichiometric dissipation rate are symbolized by θ_{st} and χ_{st} , respectively. The subscript “st” indicates the quantity at the stoichiometric value of the mixture fraction. The highest branch corresponds to the steady burning, the lowest one to the complete extinction. These two states are stable and the middle one is unstable.

Figure 2 displays the incomplete set of solutions of the flamelet equations (5), which are extracted from the library of the SLFM. It contains the two stable states but misses the unstable one in Fig. 1. The steady burning branch is located at $\theta_{st} \geq \theta_q$ and the extinction branch located at $\theta_{st} \leq \theta_e$. However, there exists a gap for $\theta_e < \theta_{st} < \theta_q$. This gap indicates the discontinuous transition of the temperature. Since temperature is an essential factor in the chemical reaction process, the existing gap would definitely affect the description of reaction process provided by the flamelet library.

Figure 3 shows the explicit dependence of reaction rate on mixture fraction at different temperatures using the SFLM library. It can be clearly observed that the reaction rate is continuously dependent on mixture fraction for temperatures larger than the quenching one, such as $\theta = 0.7$ and 0.8 . However, the reaction rate is not continuously dependent on the mixture fraction for temperatures between the extinction and quenching points, such as $\theta = 0.4, 0.5$ and 0.6 . There are gaps between the left and right parts of the $\omega_P - z$ curves for a given temperature. It shows that the reaction rates are unknown for some mixture fractions. This is not con-

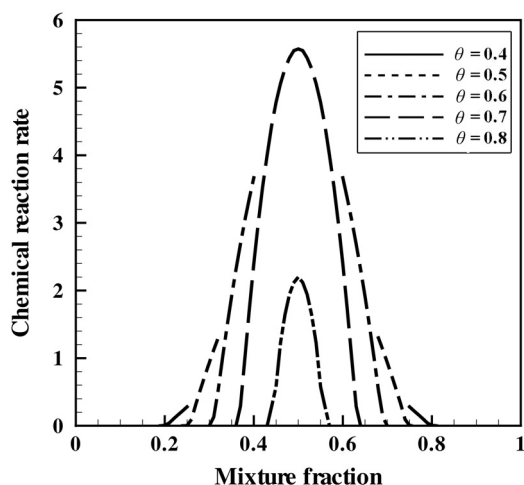


Fig. 3. The revealed relations between chemical reaction rate and temperature in the SLFM. This shows the discontinuous distributions of chemical reaction rate.

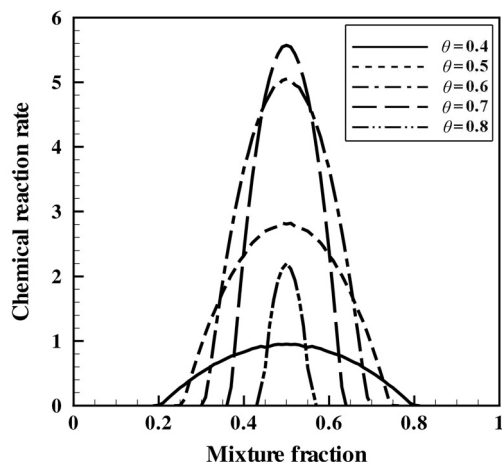


Fig. 4. The improved relations between chemical reaction rate and temperature. The continuous distribution of chemical reaction rate is obtained, which is consistent with the Arrhenius law.

sistent with the Arrhenius law. In other words, when the temperature is greater than θ_e and lower than θ_q , the reaction would suddenly stop and the flame would be globally extinguished. Therefore, the SLFM is not able to predict the local extinction and reignition.

Figure 4 plots the dependence of reaction rate on mixture fraction at different temperatures, using the complete set of solution of the flamelet equations. The gap between θ_q and θ_e in Fig. 2 was filled by using the

unstable branch in Fig. 1. The reactions are continuously dependent on the mixture fraction in response to changes in temperature without any gap. This is consistent with the Arrhenius law. Therefore, when the temperature suddenly decreases due to local extinction, subsequent reignition could take place at a lower temperature.

This result indicates the role of the unstable branch. In the proposed flamelet/progress variable method,^[11] the unstable branch delineates the border between ignition and extinction of the flame. However, Sripakagorn *et al.*^[7] applied a flame element tracking approach to investigate the time history of flame elements along the stoichiometric surface. It was shown that the unstable branch is not a border between ignition and extinction. This is in agreement with the present study. Moreover, it can be seen that the solutions on the unstable branch can fill the gap of the discontinuous curves in Fig. 3.

From the above, an implicit relation between the temperature and reaction rate in the SLFM is proposed. The reaction rate is discontinuous in the SLFM when the temperature is greater than θ_e and lower than θ_q . This is not consistent with the Arrhenius law. It suggests an explanation that the SLFM is not capable of predicting local extinction and reignition. A modification can be made by using the unstable branch. As a result, the reaction rate becomes continuous. This modification is consistent with the Arrhenius law and thus can represent local extinction and reignition.

This work was supported by CAS (KJ CX2-SW-L08), 973 Program of China (2007CB814800, 2009CB724100), NSFC (11072247, 10702074, 10732090, 50906096) and the LNM initial funding for young investigators.

1. W. E. Mell, V. Nilsen, G. Kosály, and J. J. Riley, *Phys. Fluids* **6**, 1331 (1994).
2. B. Cuenot and T. Poinso, *Proc. Combust. Inst.* **25**, 1383 (1994).
3. H. Pitsch, M. Chen, and N. Peters, *Proc. Combust. Inst.* **27**, 1057 (1998).
4. K. Claramunt, R. Cònsul, D. Carbonell, and C. D. Pérez-Segarra, *Combustion and Flame* **145**, 845 (2006).
5. R. Cònsul, A. Oliva, C. D. Pérez-Segarra, D. Carbonell, and L. P. H. de Goeij, *Combustion and Flame* **153**, 71 (2008).
6. C. D. Pierce and P. Moin, *J. Fluid Mech.* **504**, 73 (2004).
7. P. Sripakagorn, S. Mitarai, G. Kosály, and H. Pitsch, *J. Fluid Mech.* **518**, 231 (2004).
8. S. Mitarai, J. J. Riley, and G. Kosály, *Phys. Fluids* **15**, 3856 (2003).
9. S. R. Turns, *An Introduction to Combustion: Concepts and Applications* (McGraw-Hill, 1996).
10. J. Zhang, G. Jin, and G. He PSTOP/366254/SPE/256056 in press.
11. C. D. Pierce, *Progress-variable approach for large-eddy simulation of turbulent combustion*, Ph.D. thesis, Stanford.